Stability Analysis and Optimization of Transport/Reaction Systems

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We will present algorithms and applications for performing stability analysis and optimization of large-scale transport/reaction calculations. The algorithms and capabilities of the MPSalsa reacting flows code are being presented in detail in another paper by John Shadid. Of particular relevance to this paper is the fully-coupled Newton algorithm with sophisticated iterative linear solvers that lead to a robust capability for computing steady state solutions. Having the ability to apply and invert a Jacobian matrix open the door to powerful analysis and optimization tools.

A set of stability analysis algorithms for large-scale applications has been developed to perform parameter continuation, linear stability analysis, and bifurcation tracking, and collected in the LOCA library. These algorithms will be briefly presented, as will results from driving MPSalsa with LOCA on some large incompressible flow application.

Furthermore, optimization algorithms have been linked to MPSalsa that interface at the Newton iteration level. This moderately invasive approach can be much more efficient at locating optimum solutions then non-invasive decouple optimization strategies. We will present results for some large-scale PDE-constrained optimization problems.